

Dimethyl sulfoxide
67-68-5 | DTXSID2021735

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: -1.15

Global applicability domain: Inside

Local applicability domain index: 5.55e-01

Confidence level: 5.06e-01

Nearest Neighbors from the Training Set

Image not found

Dimethyl sulfoxide

Measured: -1.35

Predicted: -1.15

Image not found

Dimethyl sulfone

Measured: -1.41

Predicted: -1.07

Image not found

Thiophene, tetrahydro-, 1-oxide

Measured: -0.960

Predicted: -0.976

Image not found

Methanesulfonyl fluoride

Measured: 0.55

Predicted: 2.61e-01

Image not found

Sulfolane

Measured: -0.770

Predicted: -0.689